

Dynamics of Bose-Einstein Condensates

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Abstract

We report on some recent results concerning the dynamics of Bose-Einstein condensates, obtained in a series of joint papers [5, 6] with L. Erdős and H.-T. Yau. Starting from many body quantum dynamics, we present a rigorous derivation of a cubic nonlinear Schrödinger equation known as the Gross-Pitaevskii equation for the time evolution of the condensate wave function.

1 Introduction

Bosonic systems at very low temperature are characterized by the fact that a macroscopic fraction of the particles collapses into a single one-particle state. Although this phenomenon, known as Bose-Einstein condensation, was already predicted in the early days of quantum mechanics, the first empirical evidence for its existence was only obtained in 1995, in experiments performed by groups led by Cornell and Wieman at the University of Colorado at Boulder and by Ketterle at MIT (see [2, 4]). In these important experiments, atomic gases were initially trapped by magnetic fields and cooled down at very low temperatures. Then the magnetic traps were switched off and the consequent time evolution of the gas was observed; for sufficiently small temperatures, the particles remained close together and the gas moved as a single particle, a clear sign for the existence of condensation.

In the last years important progress has also been achieved in the theoretical understanding of Bose-Einstein condensation. In [10], Lieb, Yngvason, and Seiringer considered a trapped Bose gas consisting of N three-dimensional particles described by the Hamiltonian

$$H_N^{\text{trap}} = \sum_{j=1}^N (-\Delta_j + V_{\text{ext}}(x_j)) + \sum_{i<j}^N V_a(x_i - x_j), \quad (1.1)$$

where V_{ext} is an external confining potential and $V_a(x)$ is a repulsive interaction potential with scattering length a (here and in the rest of the paper we use the notation $\nabla_j = \nabla_{x_j}$ and $\Delta_j = \Delta_{x_j}$). Letting $N \rightarrow \infty$ and $a \rightarrow 0$ with $Na = a_0$ fixed, they showed that the ground state energy $E(N)$ of (1.1) divided by the number of particle N converges to

$$\lim_{N \rightarrow \infty, Na=a_0} \frac{E(N)}{N} = \min_{\varphi \in L^2(\mathbb{R}^3): \|\varphi\|=1} \mathcal{E}_{\text{GP}}(\varphi)$$

where \mathcal{E}_{GP} is the Gross-Pitaevskii energy functional

$$\mathcal{E}_{\text{GP}}(\varphi) = \int dx \left(|\nabla \varphi(x)|^2 + V_{\text{ext}}(x)|\varphi(x)|^2 + 4\pi a_0 |\varphi(x)|^4 \right). \quad (1.2)$$

Later, in [9], Lieb and Seiringer also proved that trapped Bose gases characterized by the Gross-Pitaevskii scaling $Na = a_0 = \text{const}$ exhibit Bose-Einstein condensation in the ground state. More precisely, they showed that, if ψ_N is the ground state wave function of the Hamiltonian (1.1) and if $\gamma_N^{(1)}$ denotes the corresponding one-particle marginal (defined as the partial trace of the density matrix $\gamma_N = |\psi_N\rangle\langle\psi_N|$ over the last $N - 1$ particles, with the convention that $\text{Tr } \gamma_N^{(1)} = 1$ for all N), then

$$\gamma_N^{(1)} \rightarrow |\phi_{\text{GP}}\rangle\langle\phi_{\text{GP}}| \quad \text{as } N \rightarrow \infty. \quad (1.3)$$

Here $\phi_{\text{GP}} \in L^2(\mathbb{R}^3)$ is the minimizer of the Gross-Pitaevskii energy functional (1.2). The interpretation of this result is straightforward; in the limit of large N , all particles, apart from a fraction vanishing as $N \rightarrow \infty$, are in the same one-particle state described by the wave-function $\phi_{\text{GP}} \in L^2(\mathbb{R}^3)$. In this sense the ground state of (1.1) exhibits complete Bose-Einstein condensation into ϕ_{GP} .

In joint works with L. Erdős and H.-T. Yau (see [5, 6, 7]), we prove that the Gross-Pitaevskii theory can also be used to describe the dynamics of Bose-Einstein condensates. In the Gross-Pitaevskii scaling (characterized by the fact that the scattering length of the interaction potential is of the order $1/N$) we show, under some conditions on the interaction potential and on the initial N -particle wave function, that complete Bose-Einstein condensation is preserved by the time evolution. Moreover we prove that the dynamics of the condensate wave function is governed by the time-dependent Gross-Pitaevskii equation associated with the energy functional (1.2).

As an example, consider the experimental set-up described above, where the dynamics of an initially confined gas is observed after removing the traps. Mathematically, the trapped gas can be described by the Hamiltonian (1.1), where the confining potential V_{ext} models the magnetic traps. When cooled down at very low temperatures, the system essentially relaxes to the ground state ψ_N of (1.1); from [9] it follows that at time $t = 0$, immediately before switching off the traps, the system exhibits complete Bose-Einstein condensation into ϕ_{GP} in the sense (1.3). At time $t = 0$ the traps are turned off, and one observes the evolution of the system generated by the translation invariant Hamiltonian

$$H_N = - \sum_{j=1}^N \Delta_j + \sum_{i < j}^N V_a(x_i - x_j).$$

Our results (stated in more details in Section 3 below) imply that, if $\psi_{N,t} = e^{-iH_N t} \psi_N$ is the time evolution of the initial wave function ψ_N and if $\gamma_{N,t}^{(1)}$ denotes the one-particle marginal associated with $\psi_{N,t}$, then, for any fixed time $t \in \mathbb{R}$,

$$\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \rightarrow \infty$$

where φ_t is the solution of the nonlinear time-dependent Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \quad (1.4)$$

with the initial data $\varphi_{t=0} = \phi_{\text{GP}}$. In other words, we prove that at arbitrary time $t \in \mathbb{R}$, the system still exhibits complete condensation, and the time-evolution of the condensate wave function is determined by the Gross-Pitaevskii equation (1.4).

The goal of this manuscript is to illustrate the main ideas of the proof of the results obtained in [5, 6, 7]. The paper is organized as follows. In Section 2 we define the model more precisely, and we give a heuristic argument to explain the emergence of the Gross-Pitaevskii equation (1.4). In Section 3 we present our main results. In Section 4 we illustrate the general strategy used to prove the main results and, finally, in Sections 5 and 6 we discuss the two most important parts of the proof in some more details.

2 Heuristic Derivation of the Gross-Pitaevskii Equation

To describe the interaction among the particles we choose a positive, spherical symmetric, compactly supported, smooth function $V(x)$. We denote the scattering length of V by a_0 .

Recall that the scattering length of V is defined by the spherical symmetric solution to the zero energy equation

$$\left(-\Delta + \frac{1}{2}V(x)\right)f(x) = 0 \quad f(x) \rightarrow 1 \quad \text{as } |x| \rightarrow \infty. \quad (2.1)$$

The scattering length of V is defined then by

$$a_0 = \lim_{|x| \rightarrow \infty} |x| - |x|f(x).$$

This limit can be proven to exist if V decays sufficiently fast at infinity. Note that, since we assumed V to have compact support, we have

$$f(x) = 1 - \frac{a_0}{|x|} \quad (2.2)$$

for $|x|$ sufficiently large. Another equivalent characterization of the scattering length is given by

$$8\pi a_0 = \int dx V(x)f(x). \quad (2.3)$$

To recover the Gross-Pitaevskii scaling, we define $V_N(x) = N^2V(Nx)$. By scaling it is clear that the scattering length of V_N equals $a = a_0/N$. In fact if $f(x)$ is the solution to (2.1), it is clear that $f_N(x) = f(Nx)$ solves

$$\left(-\Delta + \frac{1}{2}V_N(x)\right)f_N(x) = 0 \quad (2.4)$$

with the boundary condition $f_N(x) \rightarrow 1$ as $|x| \rightarrow \infty$. From (2.2), we obtain

$$f_N(x) = 1 - \frac{a_0}{N|x|} = 1 - \frac{a}{|x|}$$

for $|x|$ large enough. In particular the scattering length a of V_N is given by $a = a_0/N$.

We consider the dynamics generated by the translation invariant Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_j + \sum_{i<j}^N V_N(x_i - x_j) \quad (2.5)$$

acting on the Hilbert space $L_s^2(\mathbb{R}^{3N}, dx_1 \dots dx_N)$, the bosonic subspace of $L^2(\mathbb{R}^{3N}, dx_1 \dots dx_N)$ consisting of all permutation symmetric functions (although it is possible to extend our analysis to include an external potential, to keep the discussion as simple as possible we only consider the translation invariant case (2.5)). We consider solutions $\psi_{N,t}$ of the N -body Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}. \quad (2.6)$$

Let $\gamma_{N,t} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$ denote the density matrix associated with $\psi_{N,t}$, defined as the orthogonal projection onto $\psi_{N,t}$. In order to study the limit $N \rightarrow \infty$, we introduce the marginal densities of $\gamma_{N,t}$. For $k = 1, \dots, N$, we define the k -particle density matrix $\gamma_{N,t}^{(k)}$ associated with $\psi_{N,t}$ by taking

the partial trace of $\gamma_{N,t}$ over the last $N - k$ particles. In other words, $\gamma_{N,t}^{(k)}$ is defined as the positive trace class operator on $L_s^2(\mathbb{R}^{3k})$ with kernel given by

$$\gamma_{N,t}^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) = \int d\mathbf{x}_{N-k} \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) \overline{\psi}_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k}). \quad (2.7)$$

Here and in the rest of the paper we use the notation $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $\mathbf{x}_k = (x_1, x_2, \dots, x_k)$, $\mathbf{x}'_k = (x'_1, x'_2, \dots, x'_k)$, and $\mathbf{x}_{N-k} = (x_{k+1}, x_{k+2}, \dots, x_N)$.

We consider initial wave functions $\psi_{N,0}$ exhibiting complete condensation in a one-particle state φ . Thus at time $t = 0$, we assume that

$$\gamma_{N,0}^{(1)} \rightarrow |\varphi\rangle\langle\varphi| \quad \text{as } N \rightarrow \infty. \quad (2.8)$$

It turns out that the last equation immediately implies that

$$\gamma_{N,0}^{(k)} \rightarrow |\varphi\rangle\langle\varphi|^{\otimes k} \quad \text{as } N \rightarrow \infty \quad (2.9)$$

for every fixed $k \in \mathbb{N}$ (the argument, due to Lieb and Seiringer, can be found in [9], after Theorem 1). It is also interesting to notice that the convergence (2.8) (and (2.9)) in the trace class norm is equivalent to the convergence in the weak* topology defined on the space of trace class operators on \mathbb{R}^3 (or \mathbb{R}^{3k} , for (2.9)); we thank A. Michelangeli for pointing out this fact to us (the proof is based on general arguments, such as Grümm's Convergence Theorem).

Starting from the Schrödinger equation (2.6) for the wave function $\psi_{N,t}$, we can derive evolution equations for the marginal densities $\gamma_{N,t}^{(k)}$. The dynamics of the marginals is governed by a hierarchy of N coupled equations usually known as the BBGKY hierarchy.

$$\begin{aligned} i\partial_t \gamma_{N,t}^{(k)} &= \sum_{j=1}^N \left[-\Delta_j, \gamma_{N,t}^{(k)} \right] + \sum_{i < j}^k \left[V_N(x_i - x_j), \gamma_{N,t}^{(k)} \right] \\ &\quad + (N - k) \sum_{j=1}^k \text{Tr}_{k+1} \left[V_N(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right]. \end{aligned} \quad (2.10)$$

Here Tr_{k+1} denotes the partial trace over the $(k+1)$ -th particle.

Next we study the limit $N \rightarrow \infty$ of the density $\gamma_{N,t}^{(k)}$ for fixed $k \in \mathbb{N}$. For simplicity we fix $k = 1$. From (2.10), the evolution equation for the one-particle density matrix, written in terms of its kernel $\gamma_{N,t}^{(1)}(x_1; x'_1)$ is given by

$$\begin{aligned} i\partial_t \gamma_{N,t}^{(1)}(x_1, x'_1) &= (-\Delta_1 + \Delta'_1) \gamma_{N,t}^{(1)}(x_1; x'_1) \\ &\quad + (N - 1) \int dx_2 (V_N(x_1 - x_2) - V_N(x'_1 - x_2)) \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2). \end{aligned} \quad (2.11)$$

Suppose now that $\gamma_{\infty,t}^{(1)}$ and $\gamma_{\infty,t}^{(2)}$ are limit points (with respect to the weak* topology) of $\gamma_{N,t}^{(1)}$ and, respectively, $\gamma_{N,t}^{(2)}$ as $N \rightarrow \infty$. Since, formally,

$$(N - 1)V_N(x) = (N - 1)N^2V(Nx) \simeq N^3V(Nx) \rightarrow b_0\delta(x) \quad \text{with } b_0 = \int dx V(x)$$

as $N \rightarrow \infty$, we could naively expect the limit points $\gamma_{\infty,t}^{(1)}$ and $\gamma_{\infty,t}^{(2)}$ to satisfy the limiting equation

$$i\partial_t \gamma_{\infty,t}^{(1)}(x_1; x'_1) = (-\Delta_1 + \Delta'_1) \gamma_{\infty,t}^{(1)}(x_1; x'_1) + b_0 \int dx_2 (\delta(x_1 - x_2) - \delta(x'_1 - x_2)) \gamma_{\infty,t}^{(2)}(x_1, x_2; x'_1, x_2). \quad (2.12)$$

From (2.9) we have, at time $t = 0$,

$$\begin{aligned} \gamma_{\infty,0}^{(1)}(x_1; x'_1) &= \varphi(x_1) \bar{\varphi}(x'_1) \\ \gamma_{\infty,0}^{(2)}(x_1, x_2; x'_1, x'_2) &= \varphi(x_1) \varphi(x_2) \bar{\varphi}(x'_1) \bar{\varphi}(x'_2). \end{aligned} \quad (2.13)$$

If condensation is really preserved by the time evolution, also at time $t \neq 0$ we have

$$\begin{aligned} \gamma_{\infty,t}^{(1)}(x_1; x'_1) &= \varphi_t(x_1) \bar{\varphi}_t(x'_1) \\ \gamma_{\infty,t}^{(2)}(x_1, x_2; x'_1, x'_2) &= \varphi_t(x_1) \varphi_t(x_2) \bar{\varphi}_t(x'_1) \bar{\varphi}_t(x'_2). \end{aligned} \quad (2.14)$$

Inserting (2.14) in (2.12), we obtain the self-consistent equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + b_0 |\varphi_t|^2 \varphi_t \quad (2.15)$$

for the condensate wave function φ_t . This equation has the same form as the time-dependent Gross-Pitaevskii equation (1.4), but a different coefficient in front of the nonlinearity (b_0 instead of $8\pi a_0$).

The reason why we obtain the wrong coupling constant in (2.15) is that going from (2.11) to (2.12), we took the two limits

$$(N-1)V_N(x) \rightarrow b_0 \delta(x) \quad \text{and} \quad \gamma_{N,t}^{(2)} \rightarrow \gamma_{\infty,t}^{(2)} \quad (2.16)$$

independently from each other. However, since the scattering length of the interaction is of the order $1/N$, the two-particle density $\gamma_{N,t}^{(2)}$ develops a short scale correlation structure on the length scale $1/N$, which is exactly the same length scale on which the potential V_N varies. For this reason the two limits in (2.16) cannot be taken independently. In order to obtain the correct Gross-Pitaevskii equation (1.4) we need to take into account the correlations among the particles, and the short scale structure they create in the marginal density $\gamma_{N,t}^{(2)}$.

To describe the correlations among the particles we make use of the solution $f_N(x)$ to the zero energy scattering equation (2.4). Assuming that the function $f_N(x_i - x_j)$ gives a good approximation for the correlations between particles i and j , we may expect that the one- and two-particle densities associated with the evolution of a condensate are given, for large but finite N , by

$$\begin{aligned} \gamma_{N,t}^{(1)}(x_1; x'_1) &\simeq \varphi_t(x_1) \bar{\varphi}_t(x'_1) \\ \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x'_2) &\simeq f_N(x_1 - x_2) f_N(x'_1 - x'_2) \varphi_t(x_1) \varphi_t(x_2) \bar{\varphi}_t(x'_1) \bar{\varphi}_t(x'_2). \end{aligned} \quad (2.17)$$

Inserting this ansatz into (2.11), we obtain a new self-consistent equation

$$\begin{aligned} i\partial_t \varphi_t &= -\Delta \varphi_t + \left(\lim_{N \rightarrow \infty} (N-1) \int dx f_N(x) V_N(x) \right) |\varphi_t|^2 \varphi_t \\ &= -\Delta \varphi_t + \left(\lim_{N \rightarrow \infty} N^3 \int dx f(Nx) V(Nx) \right) |\varphi_t|^2 \varphi_t \\ &= -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \end{aligned} \quad (2.18)$$

because of (2.3). This is exactly the Gross-Pitaevskii equation (1.4), with the correct coupling constant in front of the nonlinearity.

Note that the presence of the correlation functions $f_N(x_1 - x_2)$ and $f_N(x'_1 - x'_2)$ in (2.17) does not contradict complete condensation of the system at time t . On the contrary, in the weak limit $N \rightarrow \infty$, the function f_N converges to one, and therefore $\gamma_{N,t}^{(1)}$ and $\gamma_{N,t}^{(2)}$ converge to $|\varphi_t\rangle\langle\varphi_t|$ and $|\varphi_t\rangle\langle\varphi_t|^{\otimes 2}$, respectively. The correlations described by the function f_N can only produce nontrivial effects on the macroscopic dynamics of the system because of the singularity of the interaction potential V_N .

From this heuristic argument it is clear that, in order to obtain a rigorous derivation of the Gross-Pitaevskii equation (2.18), we need to identify the short scale structure of the marginal densities and prove that, in a very good approximation, it can be described by the function f_N as in (2.17). In other words, we need to show a very strong separation of scales in the marginal density $\gamma_{N,t}^{(2)}$ (and, more generally, in the k -particle density $\gamma_{N,t}^{(k)}$) associated with the solution of the N -body Schrödinger equation; the Gross-Pitaevskii theory can only be correct if $\gamma_{N,t}^{(k)}$ has a regular part, which factorizes for large N into the product of k copies of the orthogonal projection $|\varphi_t\rangle\langle\varphi_t|$, and a time independent singular part, due to the correlations among the particles, and described by products of the functions $f_N(x_i - x_j)$, $1 \leq i, j \leq k$.

3 Main Results

To prove our main results we need to assume the interaction potential to be sufficiently weak. To measure the strength of the potential, we introduce the dimensionless quantity

$$\alpha = \sup_{x \in \mathbb{R}^3} |x|^2 V(x) + \int \frac{dx}{|x|} V(x). \quad (3.1)$$

Apart from the smallness assumption on the potential, we also need to assume that the correlations characterizing the initial N -particle wave function are sufficiently weak. We define therefore the notion of *asymptotically factorized* wave functions. We say that a family of permutation symmetric wave functions ψ_N is asymptotically factorized if there exists $\varphi \in L^2(\mathbb{R}^3)$ and, for any fixed $k \geq 1$, there exists a family $\xi_N^{(N-k)} \in L_s^2(\mathbb{R}^{3(N-k)})$ such that

$$\left\| \psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)} \right\| \rightarrow 0 \quad \text{as } N \rightarrow \infty. \quad (3.2)$$

It is simple to check that, if ψ_N is asymptotically factorized, then it exhibits complete Bose-Einstein condensation in the one-particle state φ (in the sense that the one-particle density associated with ψ_N satisfy $\gamma_N^{(1)} \rightarrow |\varphi\rangle\langle\varphi|$ as $N \rightarrow \infty$). Asymptotic factorization is therefore a stronger condition than complete condensation, and it provides more control on the correlations of ψ_N .

Theorem 3.1. *Assume that $V(x)$ is a positive, smooth, spherical symmetric, and compactly supported potential such that α (defined in (3.1)) is sufficiently small. Consider an asymptotically factorized family of wave functions $\psi_N \in L_s^2(\mathbb{R}^{3N})$, exhibiting complete Bose-Einstein condensation in a one-particle state $\varphi \in H^1(\mathbb{R}^3)$, in the sense that*

$$\gamma_N^{(1)} \rightarrow |\varphi\rangle\langle\varphi| \quad \text{as } N \rightarrow \infty \quad (3.3)$$

where $\gamma_N^{(1)}$ denotes the one-particle density associated with ψ_N . Then, for any fixed $t \in \mathbb{R}$, the one-particle density $\gamma_{N,t}^{(1)}$ associated with the solution $\psi_{N,t}$ of the N -particle Schrödinger equation (2.6) satisfies

$$\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \rightarrow \infty \quad (3.4)$$

where φ_t is the solution to the time-dependent Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t \quad (3.5)$$

with initial data $\varphi_{t=0} = \varphi$.

The convergence in (3.3) and (3.4) is in the trace norm topology (which in this case is equivalent to the weak* topology defined on the space of trace class operators on \mathbb{R}^3). Moreover, from (3.4) we also get convergence of higher marginal. For every $k \geq 1$, we have

$$\gamma_{N,t}^{(k)} \rightarrow |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{as } N \rightarrow \infty.$$

Theorem 3.1 can be used to describe the dynamics of condensates satisfying the condition of asymptotic factorization. The following two corollaries provide examples of such initial data.

The simplest example of N -particle wave function satisfying the assumption of asymptotic factorization is given by a product state.

Corollary 3.2. *Under the assumptions on $V(x)$ stated in Theorem 3.1, let $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$ for an arbitrary $\varphi \in H^1(\mathbb{R}^3)$. Then, for any $t \in \mathbb{R}$,*

$$\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \rightarrow \infty$$

where φ_t is a solution of the Gross-Pitaevskii equation (3.5) with initial data $\varphi_{t=0} = \varphi$.

The second application of Theorem 3.1 gives a mathematical description of the results of the experiments depicted in the introduction.

Let

$$H_N^{\text{trap}} = \sum_{j=1}^N (-\Delta_j + V_{\text{ext}}(x_j)) + \sum_{i<j}^N V_N(x_i - x_j) \quad (3.6)$$

with a confining potential V_{ext} . Let ψ_N be the ground state of H_N^{trap} . By [9], ψ_N exhibits complete Bose Einstein condensation into the minimizer ϕ_{GP} of the Gross-Pitaevskii energy functional \mathcal{E}_{GP} defined in (1.2). In other words

$$\gamma_N^{(1)} \rightarrow |\phi_{\text{GP}}\rangle\langle\phi_{\text{GP}}| \quad \text{as } N \rightarrow \infty.$$

In [5], we demonstrate that ψ_N also satisfies the condition (3.2) of asymptotic factorization. From this observation, we obtain the following corollary.

Corollary 3.3. *Under the assumptions on $V(x)$ stated in Theorem 3.1, let ψ_N be the ground state of (3.6), and denote by $\gamma_{N,t}^{(1)}$ the one-particle density associated with the solution $\psi_{N,t} = e^{-iH_N t}\psi_N$ of the Schrödinger equation (2.6). Then, for any fixed $t \in \mathbb{R}$,*

$$\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \rightarrow \infty$$

where φ_t is the solution of the Gross-Pitaevskii equation (3.5) with initial data $\varphi_{t=0} = \phi_{\text{GP}}$.

Although the second corollary describes physically more realistic situations, also the first corollary has interesting consequences. In Section 2, we observed that the emergence of the scattering length in the Gross-Pitaevskii equation is an effect due to the correlations. The fact that the Gross-Pitaevskii equation describes the dynamics of the condensate also if the initial wave function is completely

uncorrelated, as in Corollary 3.2, implies that the N -body Schrödinger dynamics generates the singular correlation structure in very short times. Of course, when the wave function develops correlations on the length scale $1/N$, the energy associated with this length scale decreases; since the total energy is conserved by the Schrödinger evolution, we must conclude that together with the short scale structure at scales of order $1/N$, the N -body dynamics also produces oscillations on intermediate length scales $1/N \ll \ell \ll 1$, which carry the excess energy (the difference between the energy of the factorized wave function and the energy of the wave function with correlations on the length scale $1/N$) and which have no effect on the macroscopic dynamics (because only variations of the wave function on length scales of order one and order $1/N$ affect the macroscopic dynamics described by the Gross-Pitaevskii equation).

4 General Strategy of the Proof and Previous Results

In this section we illustrate the strategy used to prove Theorem 3.1. The proof is divided into three main steps.

Step 1. Compactness of $\gamma_{N,t}^{(k)}$. Recall, from (2.7), the definition of the marginal densities $\gamma_{N,t}^{(k)}$ associated with the solution $\psi_{N,t} = \exp(-iH_N t)\psi_N$ of the N -body Schrödinger equation. By definition, for any $N \in \mathbb{N}$ and $t \in \mathbb{R}$, $\gamma_{N,t}^{(k)}$ is a positive operator in $\mathcal{L}_k^1 = \mathcal{L}^1(L^2(\mathbb{R}^{3k}))$ (the space of trace class operators on $L^2(\mathbb{R}^{3k})$) with trace equal to one. For fixed $t \in \mathbb{R}$ and $k \geq 1$, it follows by standard general argument (Banach-Alaouglu Theorem) that the sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ is compact with respect to the weak* topology of \mathcal{L}_k^1 . Note here that \mathcal{L}_k^1 has a weak* topology because $\mathcal{L}_k^1 = \mathcal{K}_k^*$, where $\mathcal{K}_k = \mathcal{K}(L^2(\mathbb{R}^{3k}))$ is the space of compact operators on $L^2(\mathbb{R}^{3k})$. To make sure that we can find subsequences of $\gamma_{N,t}^{(k)}$ which converge for all times in a certain interval, we fix $T > 0$ and consider the space $C([0, T], \mathcal{L}_k^1)$ of all functions of $t \in [0, T]$ with values in \mathcal{L}_k^1 which are continuous with respect to the weak* topology on \mathcal{L}_k^1 . Since \mathcal{K}_k is separable, it follows that the weak* topology on the unit ball of \mathcal{L}_k^1 is metrizable; this allows us to prove the equicontinuity of the densities $\gamma_{N,t}^{(k)}$, and to obtain compactness of the sequences $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ in $C([0, T], \mathcal{L}_k^1)$.

Step 2. Convergence to an infinite hierarchy. By Step 1 we know that, as $N \rightarrow \infty$, the family of marginal densities $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ has at least one limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ in $\bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ with respect to the product topology. Next, we derive evolution equations for the limiting densities $\gamma_{\infty,t}^{(k)}$. Starting from the BBGKY hierarchy (2.10) for the family $\Gamma_{N,t}$, we prove that any limit point $\Gamma_{\infty,t}$ satisfies the infinite hierarchy of equations

$$i\partial_t \gamma_{\infty,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{\infty,t}^{(k)} \right] + 8\pi a_0 \sum_{j=1}^k \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)} \right] \quad (4.1)$$

for $k \geq 1$. It is at this point, in the derivation of this infinite hierarchy, that we need to identify the singular part of the densities $\gamma_{N,t}^{(k+1)}$. The emergence of the scattering length in the second term on the right hand side of (4.1) is due to short scale structure of $\gamma_{N,t}^{(k+1)}$.

It is worth noticing that the infinite hierarchy (4.1) has a factorized solution. In fact, it is simple to see that the infinite family

$$\gamma_t^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{for } k \geq 1 \quad (4.2)$$

solves (4.1) if and only if φ_t is a solution to the Gross-Pitaevskii equation (3.5).

Step 3. Uniqueness of the solution to the infinite hierarchy. To conclude the proof of Theorem 3.1, we show that the infinite hierarchy (4.1) has a unique solution. This implies immediately that the densities $\gamma_{N,t}^{(k)}$ converge; in fact, a compact sequence with at most one limit point is always convergent. Moreover, since we know that the factorized densities (4.2) are a solution, it also follows that, for any $k \geq 1$,

$$\gamma_{N,t}^{(k)} \rightarrow |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{as } N \rightarrow \infty$$

with respect to the weak* topology of \mathcal{L}_k^1 .

Similar strategies have been used to obtain rigorous derivations of the nonlinear Hartree equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + (v * |\varphi_t|^2)\varphi_t \quad (4.3)$$

for the dynamics of initially factorized wave functions in bosonic many particle mean field models, characterized by the Hamiltonian

$$H_N^{\text{mf}} = \sum_{j=1}^N -\Delta_j + \frac{1}{N} \sum_{i<j}^N v(x_i - x_j). \quad (4.4)$$

In this context, the approach outlined above was introduced by Spohn in [11], who applied it to derive (4.3) in the case of a bounded potential v . In [8], Erdős and Yau extended Spohn's result to the case of a Coulomb interaction $v(x) = \pm 1/|x|$ (partial results for the Coulomb case, in particular the convergence to the infinite hierarchy, were also obtained by Bardos, Golse, and Mauser, see [3]). More recently, Adami, Golse, and Teta used the same approach in [1] for one-dimensional systems with dynamics generated by a Hamiltonian of the form (4.4) with an N -dependent pair potential $v_N(x) = N^\beta V(N^\beta x)$, $\beta < 1$. In the limit $N \rightarrow \infty$, they obtain the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + b_0|\varphi_t|^2\varphi_t \quad \text{with } b_0 = \int V(x)dx.$$

Notice that the Hamiltonian (2.5) has the same form as the mean field Hamiltonian (4.4), with an N -dependent pair potential $v_N(x) = N^3V(Nx)$. Of course, one may also ask what happens if we consider the mean field Hamiltonian (4.4) with the N -dependent potential $v_N(x) = N^{3\beta}V(N^\beta x)$, for $\beta \neq 1$. If $\beta < 1$, the short scale structure developed by the solution of the Schrödinger equation is still characterized by the length scale $1/N$ (because the scattering length of $N^{3\beta-1}V(N^\beta x)$ is still of order $1/N$); but this time the potential varies on much larger scales, of the order $N^{-\beta} \gg N^{-1}$. For this reason, if $\beta < 1$, the scattering length does not appear in the effective macroscopic equation ($8\pi a_0$ is replaced by $b_0 = \int dx V(x)$). In [6] (and previously in [5] for $0 < \beta < 1/2$) we prove in fact that Corollary 3.2 can be extended to include the case $0 < \beta < 1$ as follows.

Theorem 4.1. *Suppose $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$, for some $\varphi \in H^1(\mathbb{R}^3)$. Let $\psi_{N,t} = e^{-iH_{\beta,N}t}\psi_N$ with the mean-field Hamiltonian*

$$H_{\beta,N} = \sum_{j=1}^N -\Delta_j + \frac{1}{N} \sum_{i<j}^N N^{3\beta}V(N^\beta(x_i - x_j))$$

for a positive, spherical symmetric, compactly supported, and smooth potential V such that α (defined in (3.1)) is sufficiently small. Let $\gamma_{N,t}^{(1)}$ be the one-particle density associated with $\psi_{N,t}$. Then, if $0 < \beta \leq 1$ we have, for any fixed $t \in \mathbb{R}$, $\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$ as $N \rightarrow \infty$. Here φ_t is the solution to the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + \sigma|\varphi_t|^2\varphi_t$$

with initial data $\varphi_{t=0} = \varphi$ and with

$$\sigma = \begin{cases} 8\pi a_0 & \text{if } \beta = 1 \\ b_0 & \text{if } 0 < \beta < 1 \end{cases}.$$

5 Convergence to the Infinite Hierarchy

In this section we give some more details concerning Step 2 in the strategy outlined above. We consider a limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ and we prove that $\Gamma_{\infty,t}$ satisfies the infinite hierarchy (4.1). To this end we use that, for finite N , the family $\Gamma_{N,t}$ satisfies the BBGKY hierarchy (2.10), and we show the convergence of each term in (2.10) to the corresponding term in the infinite hierarchy (4.1) (the second term on the r.h.s. of (2.10) is of smaller order and can be proven to vanish in the limit $N \rightarrow \infty$).

The main difficulty consists in proving the convergence of the last term on the right hand side of (2.10) to the last term on the right hand side of (4.1). In particular, we need to show that in the limit $N \rightarrow \infty$ we can replace the potential $(N-k)N^2V(N(x_j - x_{k+1})) \simeq N^3V(Nx)$ in the last term on the r.h.s. of (2.10) by $8\pi a_0\delta(x_j - x_{k+1})$. In terms of kernels we have to prove that

$$\int dx_{k+1} (N^3V(N(x_j - x_{k+1})) - 8\pi a_0\delta(x_j - x_{k+1})) \gamma_{N,t}^{(k+1)}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1}) \rightarrow 0 \quad (5.1)$$

as $N \rightarrow \infty$. It is enough to prove the convergence (5.1) in a weak sense, after testing the expression against a smooth k -particle kernel $J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)$. Note, however, that the observable $J^{(k)}$ does not help to perform the integration over the variable x_{k+1} .

The problem here is that, formally, the N -dependent potential $N^3V(N(x_j - x_{k+1}))$ does not converge towards $8\pi a_0\delta(x_j - x_{k+1})$ as $N \rightarrow \infty$ (it converges towards $b_0\delta(x_j - x_{k+1})$, with $b_0 = \int dx V(x)$). Eq. (5.1) is only correct because of the correlations between x_j and x_{k+1} hidden in the density $\gamma_{N,t}^{(k+1)}$. Therefore, to prove (5.1), we start by factoring out the correlations explicitly, and by proving that, as $N \rightarrow \infty$,

$$\int dx_{k+1} (N^3V(N(x_j - x_{k+1}))f_N(x_j - x_{k+1}) - 8\pi a_0\delta(x_j - x_{k+1})) \frac{\gamma_{N,t}^{(k+1)}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1})}{f_N(x_j - x_{k+1})} \rightarrow 0, \quad (5.2)$$

where $f_N(x)$ is the solution to the zero energy scattering equation (2.4). Then, in a second step, we use the fact that $f_N \rightarrow 1$ in the weak limit $N \rightarrow \infty$, to prove that the ratio $\gamma_{N,t}^{(k+1)}/f_N(x_j - x_{k+1})$ converges to the same limiting density $\gamma_{\infty,t}^{(k+1)}$ as $\gamma_{N,t}^{(k+1)}$. Eq. (5.2) looks now much better than (5.1) because, formally, $N^3V(N(x_j - x_{k+1}))f_N(x_j - x_{k+1})$ does converge to $8\pi a_0\delta(x_j - x_{k+1})$. To prove that (5.2) is indeed correct, we only need some regularity of the ratio $\gamma_{N,t}^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1})/f_N(x_j - x_{k+1})$ in the variables x_j and x_{k+1} . In terms of the N -particle wave function $\psi_{N,t}$ we need regularity of $\psi_{N,t}(\mathbf{x})/f_N(x_i - x_j)$ in the variables x_i, x_j , for any $i \neq j$. To establish the required regularity we use the following energy estimate.

Proposition 5.1. *Consider the Hamiltonian H_N defined in (2.5), with a positive, spherical symmetric, smooth and compactly supported potential V . Suppose that α (defined in (3.1)) is sufficiently small. Then there exists $C = C(\alpha) > 0$ such that*

$$\langle \psi, H_N^2 \psi \rangle \geq CN^2 \int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi(\mathbf{x})}{f_N(x_i - x_j)} \right|^2. \quad (5.3)$$

for all $i \neq j$ and for all $\psi \in L_s^2(\mathbb{R}^{3N}, d\mathbf{x})$.

Making use of this energy estimate it is possible to deduce strong a-priori bounds on the solution $\psi_{N,t}$ of the Schrödinger equation (2.6). These bounds have the form

$$\int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \leq C \quad (5.4)$$

uniformly in $N \in \mathbb{N}$ and $t \in \mathbb{R}$. To prove (5.4) we use that, by (5.3), and because of the conservation of the energy along the time evolution,

$$\int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \leq CN^{-2} \langle \psi_{N,t}, H_N^2 \psi_{N,t} \rangle = CN^{-2} \langle \psi_{N,0}, H_N^2 \psi_{N,0} \rangle. \quad (5.5)$$

From (5.5) and using an approximation argument on the initial wave function to make sure that the expectation of H_N^2 at time $t = 0$ is of the order N^2 , we obtain (5.4).

The bounds (5.4) are then sufficient to prove the convergence (5.1) (using a non-standard Poincaré inequality; see Lemma 7.2 in [6]).

Remark that the a-priori bounds (5.4) do not hold true if we do not divide the solution $\psi_{N,t}$ of the Schrödinger equation by $f_N(x_i - x_j)$ (replacing $\psi_{N,t}(\mathbf{x})/f_N(x_i - x_j)$ by $\psi_N(\mathbf{x})$ the integral in (5.4) would be of order N). It is only after removing the singular factor $f_N(x_i - x_j)$ from $\psi_{N,t}(\mathbf{x})$ that we can prove useful bounds on the regular part of the wave function.

It is through the a-priori bounds (5.4) that we identify the correlation structure of the wave function $\psi_{N,t}$ and that we show that, when x_i and x_j are close to each other, $\psi_{N,t}(\mathbf{x})$ can be approximated by the time independent singular factor $f_N(x_i - x_j)$, which varies on the length scale $1/N$, multiplied with a regular part (regular in the sense that it satisfy the bounds (5.4)). It is therefore through (5.4) that we establish the strong separation of scales in the wave function $\psi_{N,t}$ and in the marginal densities $\gamma_{N,t}^{(k)}$ which is of fundamental importance for the Gross-Pitaevskii theory.

Since it is quite short and it shows why the solution $f_N(x_i - x_j)$ to the zero energy scattering equation (2.1) can be used to describe the two-particle correlations, we reproduce in the following the proof Proposition 5.1. Note that this is the only step in the proof of our main theorem where the smallness of constant α , measuring the strength of the interaction potential, is used. The positivity of the interaction potential, on the other hand, also plays an important role in many other parts of the proof.

Proof of Proposition 5.1. We decompose the Hamiltonian (2.5) as

$$H_N = \sum_{j=1}^N h_j \quad \text{with} \quad h_j = -\Delta_j + \frac{1}{2} \sum_{i \neq j} V_N(x_i - x_j).$$

For an arbitrary permutation symmetric wave function ψ and for any fixed $i \neq j$, we have

$$\langle \psi, H_N^2 \psi \rangle = N \langle \psi, h_i^2 \psi \rangle + N(N-1) \langle \psi, h_i h_j \psi \rangle \geq N(N-1) \langle \psi, h_i h_j \psi \rangle.$$

Using the positivity of the potential, we find

$$\langle \psi, H_N^2 \psi \rangle \geq N(N-1) \left\langle \psi, \left(-\Delta_i + \frac{1}{2} V_N(x_i - x_j) \right) \left(-\Delta_j + \frac{1}{2} V_N(x_i - x_j) \right) \psi \right\rangle. \quad (5.6)$$

Next, we define $\phi(\mathbf{x})$ by $\psi(\mathbf{x}) = f_N(x_i - x_j) \phi(\mathbf{x})$ (ϕ is well defined because $f_N(x) > 0$ for all $x \in \mathbb{R}^3$); note that the definition of the function ϕ depends on the choice of i, j . Then

$$\frac{1}{f_N(x_i - x_j)} \Delta_i (f_N(x_i - x_j) \phi(\mathbf{x})) = \Delta_i \phi(\mathbf{x}) + \frac{(\Delta f_N)(x_i - x_j)}{f_N(x_i - x_j)} \phi(\mathbf{x}) + \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \nabla_i \phi(\mathbf{x}).$$

From (2.1) it follows that

$$\frac{1}{f_N(x_i - x_j)} \left(-\Delta_i + \frac{1}{2} V_N(x_i - x_j) \right) f_N(x_i - x_j) \phi(\mathbf{x}) = L_i \phi(\mathbf{x})$$

and analogously

$$\frac{1}{f_N(x_i - x_j)} \left(-\Delta_j + \frac{1}{2} V_N(x_i - x_j) \right) f_N(x_i - x_j) \phi(\mathbf{x}) = L_j \phi(\mathbf{x})$$

where we defined

$$L_\ell = -\Delta_\ell + 2 \frac{\nabla_\ell f_N(x_i - x_j)}{f_N(x_i - x_j)} \nabla_\ell, \quad \text{for } \ell = i, j.$$

Remark that, for $\ell = i, j$, the operator L_ℓ satisfies

$$\int d\mathbf{x} f_N^2(x_i - x_j) L_\ell \bar{\phi}(\mathbf{x}) \psi(\mathbf{x}) = \int d\mathbf{x} f_N^2(x_i - x_j) \bar{\phi}(\mathbf{x}) L_\ell \psi(\mathbf{x}) = \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_\ell \bar{\phi}(\mathbf{x}) \nabla_\ell \psi(\mathbf{x}).$$

Therefore, from (5.6), we obtain

$$\begin{aligned} \langle \psi, H_N^2 \psi \rangle &\geq N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) L_i \bar{\phi}(\mathbf{x}) L_j \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_i L_j \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) L_j \nabla_i \phi(\mathbf{x}) \\ &\quad + N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) [\nabla_i, L_j] \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) |\nabla_j \nabla_i \phi(\mathbf{x})|^2 \\ &\quad + N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \left(\nabla_i \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \right) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_j \phi(\mathbf{x}). \end{aligned} \tag{5.7}$$

To control the second term on the right hand side of the last equation we use bounds on the function f_N , which can be derived from the zero energy scattering equation (2.1):

$$1 - C\alpha \leq f_N(x) \leq 1, \quad |\nabla f_N(x)| \leq C \frac{\alpha}{|x|}, \quad |\nabla^2 f_N(x)| \leq C \frac{\alpha}{|x|^2} \tag{5.8}$$

for constants C independent of N and of the potential V (recall the definition of the dimensionless constant α from (3.1)). Therefore, for $\alpha < 1$,

$$\begin{aligned} &\left| \int d\mathbf{x} f_N^2(x_i - x_j) \left(\nabla_i \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \right) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_j \phi(\mathbf{x}) \right| \\ &\leq C\alpha \int d\mathbf{x} \frac{1}{|x_i - x_j|^2} |\nabla_i \phi(\mathbf{x})| |\nabla_j \phi(\mathbf{x})| \\ &\leq C\alpha \int d\mathbf{x} \frac{1}{|x_i - x_j|^2} (|\nabla_i \phi(\mathbf{x})|^2 + |\nabla_j \phi(\mathbf{x})|^2) \\ &\leq C\alpha \int d\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2 \end{aligned} \tag{5.9}$$

where we used Hardy inequality. Thus, from (5.7), and using again the first bound in (5.8), we obtain

$$\langle \psi, H_N^2 \psi \rangle \geq N(N-1)(1 - C\alpha) \int d\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2$$

which implies (5.3). \square

6 Uniqueness of the Solution to the Infinite Hierarchy

In this section we discuss the main ideas used to prove the uniqueness of the solution to the infinite hierarchy (Step 3 in the strategy outlined in Section 4).

First of all, we need to specify in which class of family of densities $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1}$ we want to prove the uniqueness of the solution to the infinite hierarchy (4.1). Clearly, the proof of the uniqueness is simpler if we can restrict our attention to smaller classes. But of course, in order to apply the uniqueness result to prove Theorem 3.1, we need to make sure that any limit point of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ is in the class for which we can prove uniqueness.

We are going to prove uniqueness for all families $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \bigoplus C([0, T], \mathcal{L}_k^1)$ with

$$\|\gamma_t^{(k)}\|_{\mathcal{H}_k} := \text{Tr} \left| (1 - \Delta_1)^{1/2} \dots (1 - \Delta_k)^{1/2} \gamma_t^{(k)} (1 - \Delta_k)^{1/2} \dots (1 - \Delta_1)^{1/2} \right| \leq C^k \quad (6.1)$$

for all $t \in [0, T]$ and for all $k \geq 1$ (with a constant C independent of k).

The following proposition guarantees that any limit point of the sequence $\Gamma_{N,t}$ satisfies (6.1).

Proposition 6.1. *Assume the same conditions as in Proposition 5.1. Suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ is a limit point of $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ with respect to the product topology on $\bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$. Then $\gamma_{\infty,t}^{(k)} \geq 0$ and there exists a constant C such that*

$$\text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{\infty,t}^{(k)} \leq C^k \quad (6.2)$$

for all $k \geq 1$ and $t \in [0, T]$.

Because of Proposition 6.1, it is enough to prove the uniqueness of the infinite hierarchy (4.1) in the following sense.

Theorem 6.2. *Suppose that $\Gamma = \{\gamma^{(k)}\}_{k \geq 1}$ is such that*

$$\|\gamma^{(k)}\|_{\mathcal{H}_k} \leq C^k \quad (6.3)$$

for all $k \geq 1$ (the norm $\|\cdot\|_{\mathcal{H}_k}$ is defined in (6.1)). Then there exists at most one solution $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \bigoplus C([0, T], \mathcal{L}_k)$ of (4.1) such that $\Gamma_{t=0} = \Gamma$ and

$$\|\gamma_t^{(k)}\|_{\mathcal{H}_k} \leq C^k \quad (6.4)$$

for all $k \geq 1$ and all $t \in [0, T]$ (with the same constant C as in (6.3)).

In the next two subsections we explain the main ideas of the proofs of Proposition 6.1 and Theorem 6.2.

6.1 Higher Order Energy Estimates

The main difficulty in proving Proposition 6.1 is the fact that the estimate (6.2) does not hold true if we replace $\gamma_{\infty,t}^{(k)}$ by the marginal density $\gamma_{N,t}^{(k)}$. More precisely,

$$\text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{N,t}^{(k)} \leq C^k \quad (6.5)$$

cannot hold true with a constant C independent of N . In fact, for finite N and $k > 1$, the k -particle density $\gamma_{N,t}^{(k)}$ still contains the short scale structure due to the correlations among the particles.

Therefore, when we take derivatives of $\gamma_{N,t}^{(k)}$ as in (6.5), the singular structure (which varies on a length scale of order $1/N$) generates contributions which diverge in the limit $N \rightarrow \infty$.

To overcome this problem, we cutoff the wave function $\psi_{N,t}$ when two or more particles come at distances smaller than some intermediate length scale ℓ , with $N^{-1} \ll \ell \ll 1$ (more precisely, the cutoff will be effective only when one or more particles come close to one of the variable x_j over which we want to take derivatives). For fixed $j = 1, \dots, N$, we define $\theta_j \in C^\infty(\mathbb{R}^{3N})$ such that

$$\theta_j(\mathbf{x}) \simeq \begin{cases} 1 & \text{if } |x_i - x_j| \gg \ell \text{ for all } i \neq j \\ 0 & \text{if there exists } i \neq j \text{ with } |x_i - x_j| \lesssim \ell \end{cases}.$$

It is important, for our analysis, that θ_j controls its derivatives (in the sense that, for example, $|\nabla_i \theta_j| \leq C\ell^{-1}\theta_j^{1/2}$); for this reason we cannot use standard compactly supported cutoffs, but instead we have to construct appropriate functions which decay exponentially when particles come close together. Making use of the functions $\theta_j(\mathbf{x})$, we prove the following higher order energy estimates.

Proposition 6.3. *Choose $\ell \ll 1$ such that $N\ell^2 \gg 1$. Suppose that α is small enough. Then there exist constants C_1 and C_2 such that, for any $\psi \in L_s^2(\mathbb{R}^{3N})$,*

$$\langle \psi, (H_N + C_1 N)^k \psi \rangle \geq C_2 N^k \int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_{k-1}(\mathbf{x}) |\nabla_1 \dots \nabla_k \psi(\mathbf{x})|^2. \quad (6.6)$$

The meaning of the bounds (6.6) is clear. We can control the L^2 -norm of the k -th derivative $\nabla_1 \dots \nabla_k \psi$ by the expectation of the k -th power of the energy per particle, if we only integrate over configurations where the first $k-1$ particles are “isolated” (in the sense that there is no particle at distances smaller than ℓ from x_1, x_2, \dots, x_{k-1}). In this sense the energy estimate in Proposition 5.1 (which, compared with Proposition 6.3, is restricted to $k=2$) is more precise than (6.6), because it identifies and controls the singularity of the wave function exactly in the region cutoff from the integral on the right side of (6.6). The point is that, while Proposition 5.1 is used to identify the two-particle correlations in the marginal densities $\gamma_{N,t}^{(k)}$ (which are essential for the emergence of the scattering length a_0 in the infinite hierarchy (4.1)), we only need Proposition 6.3 to establish properties of the limiting densities; this is why we can introduce cutoffs in (6.6), provided we can show their effect to vanish in the limit $N \rightarrow \infty$.

Note that we can allow one “free derivative”; in (6.6) we take the derivative over x_k although there is no cutoff $\theta_k(\mathbf{x})$. The reason is that the correlation structure becomes singular, in the L^2 -sense, only when we derive it twice (if one uses the zero energy solution f_N introduced in (2.1) to describe the correlations, this can be seen by observing that $\nabla f_N(x) \simeq 1/|x|$, which is locally square integrable). Remark that the condition $N\ell^2 \gg 1$ is a consequence of the fact that, if ℓ is too small, the error due to the localization of the kinetic energy on distances of order ℓ cannot be controlled. The proof of Proposition 6.3 is based on induction over k ; for details see Section 9 in [6].

From the estimates (6.6), using the preservation of the expectation of H_N^k along the time evolution and a regularization of the initial N -particle wave function ψ_N , we obtain the following bounds for the solution $\psi_{N,t} = e^{-iH_N t} \psi_N$ of the Schrödinger equation (2.6).

$$\int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_{k-1}(\mathbf{x}) |\nabla_1 \dots \nabla_k \psi_{N,t}(\mathbf{x})|^2 \leq C^k \quad (6.7)$$

uniformly in N and t , and for all $k \geq 1$. Translating these bounds in the language of the density matrix $\gamma_{N,t}$, we obtain

$$\text{Tr } \theta_1 \dots \theta_{k-1} \nabla_1 \dots \nabla_k \gamma_{N,t} \nabla_1^* \dots \nabla_k^* \leq C^k. \quad (6.8)$$

The idea now is to use the freedom in the choice of the cutoff length ℓ . If we fix the position of all particles but x_j , it is clear that the cutoff θ_j is effective in a volume at most of the order $N\ell^3$. If we choose now ℓ such that $N\ell^3 \rightarrow 0$ as $N \rightarrow \infty$ (which is of course compatible with the condition that $N\ell^2 \gg 1$), then we can expect that, in the limit of large N , the cutoff becomes negligible. This approach yields in fact the desired results; starting from (6.8), and choosing ℓ such that $N\ell^3 \ll 1$, we can complete the proof of Proposition 6.1 (see Proposition 6.3 in [6] for more details).

6.2 Expansion in Feynman Graphs

To prove Theorem 6.2, we start by rewriting the infinite hierarchy (4.1) in the integral form

$$\begin{aligned}\gamma_t &= \mathcal{U}^{(k)}(t)\gamma_0 + 8i\pi a_0 \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_s^{(k+1)} \right] \\ &= \mathcal{U}^{(k)}(t)\gamma_0 + \int_0^t ds \mathcal{U}^{(k)}(t-s) B^{(k)} \gamma_s^{(k+1)},\end{aligned}\tag{6.9}$$

where $\mathcal{U}^{(k)}(t)$ denotes the free evolution of k particles,

$$\mathcal{U}^{(k)}(t)\gamma^{(k)} = e^{it \sum_{j=1}^k \Delta_j} \gamma^{(k)} e^{-it \sum_{j=1}^k \Delta_j}$$

and the collision operator $B^{(k)}$ maps $(k+1)$ -particle operators into k -particle operators according to

$$B^{(k)}\gamma^{(k+1)} = 8i\pi a_0 \sum_{j=1}^k \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma^{(k+1)} \right]\tag{6.10}$$

(recall that Tr_{k+1} denotes the partial trace over the $(k+1)$ -th particle).

Iterating (6.9) n times we obtain the Duhamel type series

$$\gamma_t^{(k)} = \mathcal{U}^{(k)}(t)\gamma_0^{(k)} + \sum_{m=1}^{n-1} \xi_{m,t}^{(k)} + \eta_{n,t}^{(k)}\tag{6.11}$$

with

$$\begin{aligned}\xi_{m,t}^{(k)} &= \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) B^{(k+1)} \dots B^{(k+m-1)} \mathcal{U}^{(k+m)}(s_m) \gamma_0^{(k+m)} \\ &= \sum_{j_1=1}^k \sum_{j_2=1}^{k+1} \dots \sum_{j_m=1}^{k+m} \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1) \text{Tr}_{k+1} \left[\delta(x_{j_1} - x_{k+1}), \right. \\ &\quad \left. \mathcal{U}^{(k+1)}(s_1-s_2) \text{Tr}_{k+2} \left[\delta(x_{j_2} - x_{k+2}), \dots \text{Tr}_{k+m} \left[\delta(x_{j_m} - x_{k+m}), \mathcal{U}^{(k+m)}(s_m) \gamma_0^{(k+m)} \right] \dots \right] \right]\end{aligned}\tag{6.12}$$

and the error term

$$\eta_{n,t}^{(k)} = \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) B^{(k+1)} \dots B^{(k+n-1)} \gamma_{s_n}^{(k+m)}.\tag{6.13}$$

Note that the error term (6.13) has exactly the same form as the terms in (6.12), with the only difference that the last free evolution is replaced by the full evolution $\gamma_{s_n}^{(k+m)}$.

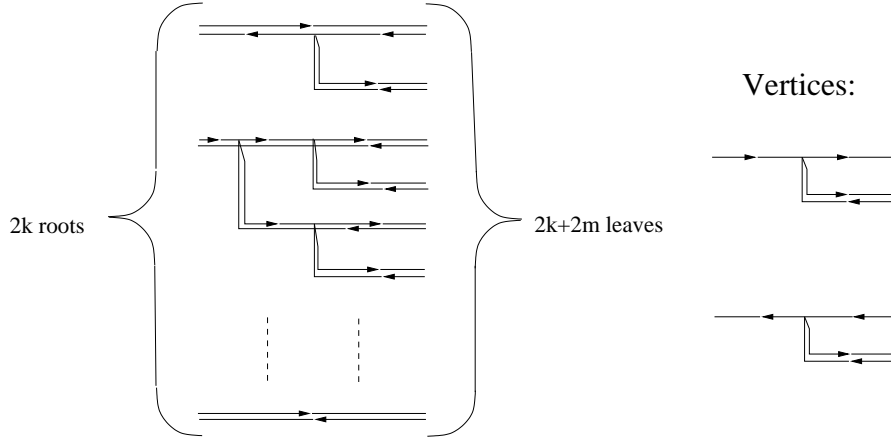


Figure 1: A Feynman graph in $\mathcal{F}_{m,k}$ and its two types of vertices

To prove the uniqueness of the infinite hierarchy, it is enough to prove that the error term (6.13) converges to zero as $n \rightarrow \infty$ (in some norm, or even only after testing it against a sufficiently large class of smooth observables). The main problem here is that the delta function in the collision operator $B^{(k)}$ cannot be controlled by the kinetic energy (in the sense that, in three dimensions, the operator inequality $\delta(x) \leq C(1 - \Delta)$ does not hold true). For this reason, the a-priori estimates $\|\gamma_t^{(k)}\|_{\mathcal{H}_k} \leq C^k$ are not sufficient to show that (6.13) converges to zero, as $n \rightarrow \infty$. Instead, we have to make use of the smoothing effects of the free evolutions $\mathcal{U}^{(k+j)}(s_j - s_{j+1})$ in (6.13) (in a similar way, Strichartz estimates are used to prove the well-posedness of nonlinear Schrödinger equations). To this end, we rewrite each term in the series (6.11) as a sum of contributions associated with certain Feynman graphs, and then we prove the convergence of the Duhamel expansion by controlling each contribution separately.

The details of the diagrammatic expansion can be found in Section 9 of [5]. Here we only present the main ideas. We start by considering the term $\xi_{m,t}^{(k)}$ in (6.12). After multiplying it with a compact k -particle observable $J^{(k)}$ and taking the trace, we expand the result as

$$\text{Tr } J^{(k)} \xi_{m,t}^{(k)} = \sum_{\Lambda \in \mathcal{F}_{m,k}} K_{\Lambda,t} \quad (6.14)$$

where $K_{\Lambda,t}$ is the contribution associated with the Feynman graph Λ . Here $\mathcal{F}_{m,k}$ denotes the set of all graphs consisting of $2k$ disjoint, paired, oriented, and rooted trees with m vertices. An example of a graph in $\mathcal{F}_{m,k}$ is drawn in Figure 1. Each vertex has one of the two forms drawn in Figure 1, with one “father”-edge on the left (closer to the root of the tree) and three “son”-edges on the right. One of the son edge is marked (the one drawn on the same level as the father edge; the other two son edges are drawn below). Graphs in $\mathcal{F}_{m,k}$ have $2k + 3m$ edges, $2k$ roots (the edges on the very left), and $2k + 2m$ leaves (the edges on the very right). It is possible to show that the number of different graphs in $\mathcal{F}_{m,k}$ is bounded by 2^{4m+k} .

The particular form of the graphs in $\mathcal{F}_{m,k}$ is due to the quantum mechanical nature of the expansion; the presence of a commutator in the collision operator (6.10) implies that, for every $B^{(k+j)}$ in (6.12), we can choose whether to write the interaction on the left or on the right of the density. When we draw the corresponding vertex in a graph in $\mathcal{F}_{m,k}$, we have to choose whether to attach it on the incoming or on the outgoing edge.

Graphs in $\mathcal{F}_{m,k}$ are characterized by a natural partial ordering among the vertices ($v \prec v'$ if the vertex v is on the path from v' to the roots); there is, however, no total ordering. The absence of total ordering among the vertices is the consequence of a rearrangement of the summands on the r.h.s. of (6.12); by removing the order between times associated with non-ordered vertices we significantly reduce the number of terms in the expansion. In fact, while (6.12) contains $(m+k)!/k!$ summands, in (6.14) we are only summing over 2^{4m+k} contributions. The price we have to pay is that the apparent gain of a factor $1/m!$ because of the ordering of the time integrals in (6.12) is lost in the new expansion (6.14). However, since the time integrations are already needed to smooth out singularities, and since they cannot be used simultaneously for smoothing and for gaining a factor $1/m!$, it seems very difficult to make use of the apparent factor $1/m!$ in (6.12). In fact, we find that the expansion (6.14) is better suited for analyzing the cumulative space-time smoothing effects of the multiple free evolutions than (6.12).

Because of the pairing of the $2k$ trees, there is a natural pairing between the $2k$ roots of the graph. Moreover, it is also possible to define a natural pairing of the leaves of the graph (this is evident in Figure 1); two leaves ℓ_1 and ℓ_2 are paired if there exists an edge e_1 on the path from ℓ_1 back to the roots, and an edge e_2 on the path from ℓ_2 to the roots, such that e_1 and e_2 are the two unmarked son-edges of the same vertex (or, if there is no unmarked sons in the path from ℓ_1 and ℓ_2 to the roots, if the two roots connected to ℓ_1 and ℓ_2 are paired).

For $\Lambda \in \mathcal{F}_{m,k}$, we denote by $E(\Lambda)$, $V(\Lambda)$, $R(\Lambda)$ and $L(\Lambda)$ the set of all edges, vertices, roots and, respectively, leaves in the graph Λ . For every edge $e \in E(\Lambda)$, we introduce a three-dimensional momentum variable p_e and a one-dimensional frequency variable α_e . Then, denoting by $\hat{\gamma}_0^{(k+m)}$ and by $\hat{J}^{(k)}$ the kernels of the density $\gamma_0^{(k+m)}$ and of the observable $J^{(k)}$ in Fourier space, the contribution $K_{\Lambda,t}$ in (6.14) is given by

$$K_{\Lambda,t} = \int \prod_{e \in E(\Lambda)} \frac{dp_e d\alpha_e}{\alpha_e - p_e^2 + i\tau_e \mu_e} \prod_{v \in V(\Lambda)} \delta \left(\sum_{e \in v} \pm \alpha_e \right) \delta \left(\sum_{e \in v} \pm p_e \right) \\ \times \exp \left(-it \sum_{e \in R(\Lambda)} \tau_e (\alpha_e + i\tau_e \mu_e) \right) \hat{J}^{(k)}(\{p_e\}_{e \in R(\Lambda)}) \hat{\gamma}_0^{(k+m)}(\{p_e\}_{e \in L(\Lambda)}) . \quad (6.15)$$

Here $\tau_e = \pm 1$, according to the orientation of the edge e . We observe from (6.15) that the momenta of the roots of Λ are the variables of the kernel of $J^{(k)}$, while the momenta of the leaves of Λ are the variables of the kernel of $\gamma_0^{(k+m)}$ (this also explain why roots and leaves of Λ need to be paired).

The denominators $(\alpha_e - p_e^2 + i\tau_e \mu_e)^{-1}$ are called propagators; they correspond to the free evolutions in the expansion (6.12) and they enter the expression (6.15) through the formula

$$e^{itp^2} = \int_{-\infty}^{\infty} d\alpha \frac{e^{it(\alpha + i\mu)}}{\alpha - p^2 + i\mu}$$

(here and in (6.15) the measure $d\alpha$ is defined by $d\alpha = d'\alpha/(2\pi i)$ where $d'\alpha$ is the Lebesgue measure on \mathbb{R}).

The regularization factors μ_e in (6.15) have to be chosen such that $\mu_{\text{father}} = \sum_{e=\text{son}} \mu_e$ at every vertex. The delta-functions in (6.15) express momentum and frequency conservation (the sum over $e \in v$ denotes the sum over all edges adjacent to the vertex v ; here $\pm \alpha_e = \alpha_e$ if the edge points towards the vertex, while $\pm \alpha_e = -\alpha_e$ if the edge points out of the vertex, and analogously for $\pm p_e$).

An analogous expansion can be obtained for the error term $\eta_{n,t}^{(k)}$ in (6.13). The problem now is to analyze the integral (6.15) (and the corresponding integral for the error term). Through an appropriate choice of the regularization factors μ_e one can extract the time dependence of $K_{\Lambda,t}$ and show that

$$|K_{\Lambda,t}| \leq C^{k+m} t^{m/4} \int \prod_{e \in E(\Gamma)} \frac{d\alpha_e dp_e}{\langle \alpha_e - p_e^2 \rangle} \prod_{v \in V(\Gamma)} \delta \left(\sum_{e \in v} \pm \alpha_e \right) \delta \left(\sum_{e \in v} \pm p_e \right) \times \left| \hat{J}^{(k)}(\{p_e\}_{e \in R(\Gamma)}) \right| \left| \hat{\gamma}_0^{(k+m)}(\{p_e\}_{e \in L(\Gamma)}) \right| \quad (6.16)$$

where we introduced the notation $\langle x \rangle = (1 + x^2)^{1/2}$.

Because of the singularity of the interaction at zero, we may be faced here with an ultraviolet problem; we have to show that all integrations in (6.16) are finite in the regime of large momenta and large frequency. Because of (6.3), we know that the kernel $\hat{\gamma}_0^{(k+m)}(\{p_e\}_{e \in L(\Lambda)})$ in (6.16) provides decay in the momenta of the leaves. From (6.3) we have, in momentum space,

$$\int dp_1 \dots dp_n (p_1^2 + 1) \dots (p_n^2 + 1) \hat{\gamma}_0^{(n)}(p_1, \dots, p_n; p_1, \dots, p_n) \leq C^n$$

for all $n \geq 1$. Power counting implies that

$$|\hat{\gamma}_0^{(k+m)}(\{p_e\}_{e \in L(\Lambda)})| \lesssim \prod_{e \in L(\Lambda)} \langle p_e \rangle^{-5/2}. \quad (6.17)$$

Using this decay in the momenta of the leaves and the decay of the propagators $\langle \alpha_e - p_e^2 \rangle^{-1}$, $e \in E(\Lambda)$, we can prove the finiteness of all the momentum and frequency integrals in (6.15). Heuristically, this can be seen using a simple power counting argument. Fix $\kappa \gg 1$, and cutoff all momenta $|p_e| \geq \kappa$ and all frequencies $|\alpha_e| \geq \kappa^2$. Each p_e -integral scales then as κ^3 , and each α_e -integral scales as κ^2 . Since we have $2k + 3m$ edges in Λ , we have $2k + 3m$ momentum- and frequency integrations. However, because of the m delta functions (due to momentum and frequency conservation), we effectively only have to perform $2k + 2m$ momentum- and frequency-integrations. Therefore the whole integral in (6.15) carries a volume factor of the order $\kappa^{5(2k+2m)} = \kappa^{10k+10m}$. Now, since there are $2k + 2m$ leaves in the graph Λ , the estimate (6.17) guarantees a decay of the order $\kappa^{-5/2(2k+2m)} = \kappa^{-5k-5m}$. The $2k + 3m$ propagators, on the other hand, provide a decay of the order $\kappa^{-2(2k+3m)} = \kappa^{-4k-6m}$. Choosing the observable $J^{(k)}$ so that $\hat{J}^{(k)}$ decays sufficiently fast at infinity, we can also gain an additional decay κ^{-6k} . Since

$$\kappa^{10k+10m} \cdot \kappa^{-5k-5m-4k-6m-6k} = \kappa^{-m-5k} \ll 1$$

for $\kappa \gg 1$, we can expect (6.15) to converge in the large momentum and large frequency regime. Remark the importance of the decay provided by the free evolution (through the propagators); without making use of it, we would not be able to prove the uniqueness of the infinite hierarchy.

This heuristic argument is clearly far from rigorous. To obtain a rigorous proof, we use an integration scheme dictated by the structure of the graph Λ ; we start by integrating the momenta and the frequency of the leaves (for which (6.17) provides sufficient decay). The point here is that when we perform the integrations over the momenta of the leaves we have to propagate the decay to the next edges on the left. We move iteratively from the right to the left of the graph, until we reach the roots; at every step we integrate the frequencies and momenta of the son edges of a fixed vertex and as a result we obtain decay in the momentum of the father edge. When we reach the roots, we use the decay of the kernel $\hat{J}^{(k)}$ to complete the integration scheme. In a typical step, we

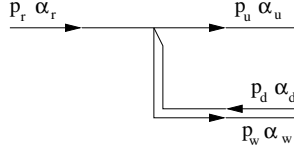


Figure 2: Integration scheme: a typical vertex

consider a vertex as the one drawn in Figure 2 and we assume to have decay in the momenta of the three son-edges, in the form $|p_e|^{-\lambda}$, $e = u, d, w$ (for some $2 < \lambda < 5/2$). Then we integrate over the frequencies $\alpha_u, \alpha_d, \alpha_w$ and the momenta p_u, p_d, p_w of the son-edges and as a result we obtain a decaying factor $|p_r|^{-\lambda}$ in the momentum of the father edge. In other words, we prove bounds of the form

$$\int \frac{d\alpha_u d\alpha_d d\alpha_w dp_u dp_d dp_w}{|p_u|^\lambda |p_d|^\lambda |p_w|^\lambda} \frac{\delta(\alpha_r = \alpha_u + \alpha_d - \alpha_w) \delta(p_r = p_u + p_d - p_w)}{\langle \alpha_u - p_u^2 \rangle \langle \alpha_d - p_d^2 \rangle \langle \alpha_w - p_w^2 \rangle} \leq \frac{\text{const}}{|p_r|^\lambda}. \quad (6.18)$$

Power counting implies that (6.18) can only be correct if $\lambda > 2$. On the other hand, to start the integration scheme we need $\lambda < 5/2$ (from (6.17) this is the decay in the momenta of the leaves, obtained from the a-priori estimates). It turns out that, choosing $\lambda = 2 + \varepsilon$ for a sufficiently small $\varepsilon > 0$, (6.18) can be made precise, and the integration scheme can be completed.

After integrating all the frequency and momentum variables, from (6.16) we obtain that

$$|K_{\Lambda, t}| \leq C^{k+m} t^{m/4}$$

for every $\Lambda \in \mathcal{F}_{m, k}$. Since the number of diagrams in $\mathcal{F}_{m, k}$ is bounded by C^{k+m} , it follows immediately that

$$\left| \text{Tr } J^{(k)} \xi_{m, t}^{(k)} \right| \leq C^{k+m} t^{m/4}.$$

Note that, from (6.12), one may expect $\xi_{m, t}^{(k)}$ to be proportional to t^m . The reason why we only get a bound proportional to $t^{m/4}$ is that we effectively use part of the time integration to control the singularity of the potentials.

Note that the only property of $\gamma_0^{(k+m)}$ used in the analysis of (6.15) is the estimate (6.3), which provides the necessary decay in the momenta of the leaves. However, since the a-priori bound (6.4) hold uniformly in time, we can use a similar argument to bound the contribution arising from the error term $\eta_{n, t}^{(k)}$ in (6.13) (as explained above, also $\eta_{n, t}^{(k)}$ can be expanded analogously to (6.14), with contributions associated to Feynman graphs similar to (6.15); the difference, of course, is that these contributions will depend on $\gamma_s^{(k+n)}$ for all $s \in [0, t]$, while (6.15) only depends on the initial data). Thus, we also obtain

$$\left| \text{Tr } J^{(k)} \eta_{n, t}^{(k)} \right| \leq C^{k+n} t^{n/4}. \quad (6.19)$$

This bound immediately implies the uniqueness. In fact, given two solutions $\Gamma_{1, t} = \{\gamma_{1, t}^{(k)}\}_{k \geq 1}$ and $\Gamma_{2, t} = \{\gamma_{2, t}^{(k)}\}_{k \geq 1}$ of the infinite hierarchy (4.1), both satisfying the a-priori bounds (6.4) and with the same initial data, we can expand both in a Duhamel series of order n as in (6.11). If we fix $k \geq 1$, and consider the difference between $\gamma_{1, t}^{(k)}$ and $\gamma_{2, t}^{(k)}$, all terms (6.12) cancel out because they only depend on the initial data. Therefore, from (6.19), we immediately obtain that, for arbitrary (sufficiently smooth) compact k -particle operators $J^{(k)}$,

$$\left| \text{Tr } J^{(k)} \left(\gamma_{1, t}^{(k)} - \gamma_{2, t}^{(k)} \right) \right| \leq 2 C^{k+n} t^{n/4}$$

Since it is independent of n , the left side has to vanish for all $t < 1/C^4$. This proves uniqueness for short times. But then, since the a-priori bounds hold uniformly in time, the argument can be repeated to prove uniqueness for all times.

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